

Beyond J_{crit} : a critical curve for suppression of H_2 -cooling in protogalaxies

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ABSTRACT

Suppression of H_2 -cooling in early protogalaxies has important implications for the formation of supermassive black holes seeds, the first generation of stars, and the epoch of reionization. This suppression can occur via photodissociation of H_2 (by ultraviolet Lyman–Werner [LW] photons) or by photodetachment of H^- , a precursor in H_2 formation (by infrared [IR] photons). Previous studies have typically adopted idealised spectra, with a blackbody or a power-law shape, in modeling the chemistry of metal-free protogalaxies, and utilised a single parameter, the critical UV flux, or J_{crit} , to determine whether H_2 -cooling is prevented. This can be misleading, and that independent of the spectral shape, there is a critical curve in the $(k_{\text{LW}}, k_{\text{H}^-})$ plane, where k_{LW} and k_{H^-} are the H_2 -dissociation rates by LW and IR photons, which determines whether a protogalaxy can cool below ~ 1000 Kelvin. We use a one-zone model to follow the chemical and thermal evolution of gravitationally collapsing protogalactic gas, to compute this critical curve, and provide an accurate analytical fit for it. We improve on previous works by considering a variety of more realistic Pop III or Pop II-type spectra from population synthesis models and perform fully frequency-dependent calculations of the H_2 -photodissociation rates for each spectrum. We compute the ratio $k_{\text{LW}}/k_{\text{H}^-}$ for each spectrum, as well as the minimum stellar mass M_* , for various IMFs and metallicities, required to prevent cooling in a neighboring halo a distance d away. We provide critical M_*/d^2 values for suppression of H_2 -cooling, with analytic fits, which can be used in future studies.

Key words: cosmology: theory – early Universe – galaxies: formation – molecular processes – stars: Population III

1 INTRODUCTION

It has long been known that the cooling of metal-free, primordial gas, from which the first generation of stars form in the first protogalaxies, is dominated by H_2 molecules (Saslaw & Zipoy 1967). Furthermore, the abundance of H_2 molecules in an early protogalaxy is sensitive to radiation impinging on the galaxy, and can be regulated by the early ultraviolet (UV) background in the Lyman–Werner bands (Haiman et al. 1997). For unusually soft spectra, infrared (IR) radiation can also play a role, through the photodetachment of the H^- ions, the main catalyst for H_2 formation in primordial gas (e.g. Omukai 2001). Recent simulations have suggested that the first stars may not be as massive as had previously been thought (e.g. Greif et al. 2011). In the extreme case that the typical first-generation stars had masses as low as a few M_\odot , the IR radiation

from these low-mass stars would dominate radiative feedback and H_2 chemistry in protogalaxies in the early Universe (Wolcott-Green & Haiman 2012).¹

In recent years, the suppression of H_2 cooling via radiative feedback has attracted a lot of attention, in the context of forming massive black hole seeds in the early universe. Observations of high-redshift quasars reveal that supermassive black holes (SMBHs) with masses of $\sim 10^9 M_\odot$ have already formed as early as redshift $z \sim 7$ (Mortlock et al. 2011). A promising way to form such early massive SMBHs is to begin with a massive (say, $\sim 10^5 M_\odot$) seed BH at redshift $z \gtrsim 10$. This massive seed can then grow further by accretion, and reach $10^9 M_\odot$ by redshift $z \sim 7$. In particular, in contrast to starting with a stellar-mass BH, the accretion rate then need not exceed the value implied by the Eddington limit

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¹ We do not consider X-rays in this paper, which can also be important for early H_2 chemistry (Haiman et al. 2000; Inayoshi & Tanaka 2015).

(see recent reviews by Volonteri & Bellovary 2012; Haiman 2013; Natarajan 2014 and Inayoshi et al. 2016).

A promising site for forming such massive BH seeds are in the nuclei of so-called atomic-cooling halos – i.e. dark matter halos with virial temperatures $T_{\text{vir}} \gtrsim 10^4 \text{K}$, or masses of $\gtrsim \text{few} \times 10^7 M_{\odot}$. Assuming that the gas at the center of such a halo is metal-free (or with metallicity at most $\sim 10^{-4}$ of the solar value; Omukai et al. 2008), and also that H_2 -cooling is disabled, the gas remains at temperatures near 10^4K . This leads to accretion rates in the core of the halo as high as $\sim 0.1 - 1 M_{\odot} \text{yr}^{-1}$. Several works have argued that under these conditions, fragmentation and Population III star-formation may be avoided, and a massive seed BH is produced instead, either by direct collapse, or via an intermediate state of a supermassive star (Oh & Haiman 2002; Bromm & Loeb 2003; Koushiappas et al. 2004; Lodato & Natarajan 2006; Spaans & Silk 2006; Begelman et al. 2006; Volonteri et al. 2008; Wise & Abel 2008; Regan & Haehnelt 2009b; Schleicher et al. 2010; Shang et al. 2010; Wolcott-Green & Haiman 2011; Wolcott-Green et al. 2011; Latif et al. 2014).²

A crucial assumption in these scenarios is the lack of H_2 -cooling. In the presence of H_2 , the gas in the atomic cooling halos would likely fragment and form Population III stars, similar to the case of lower-mass “mini-halos” (Abel et al. 2002; Bromm et al. 2002; Yoshida et al. 2003). It has been well-established in both semi-analytic studies and three-dimensional simulations that a sufficiently strong dissociating LW flux can suppress H_2 -cooling entirely, keeping the gas close to the virial temperature of the halo throughout the initial stages of collapse (Omukai 2001; Bromm & Loeb 2003; Regan & Haehnelt 2009a; Schleicher et al. 2010; Shang et al. 2010). As demonstrated in these papers, the spectral shape of the incident radiation is important in determining whether this scenario is plausible.

In nearly all previous studies, the incident radiation field is modeled either as a power-law, or as a blackbody spectrum with temperature $10^4 \leq T_*/\text{K} \leq 10^5$, and a critical flux J_{crit} is defined as the minimum intensity required to prevent cooling. Quoted at the Lyman-limit, J_{crit} for a $T_* = 10^5 \text{K}$ blackbody (hereafter referred to as T5) is usually found to be in the range $10^3 - 10^4$ in the customary J_{21} units $J(13.6\text{eV}) = J_{21} \times 10^{-21} \text{ergs}^{-1} \text{Hz}^{-1} \text{cm}^{-2} \text{sr}^{-1}$.

For the softest blackbody spectra considered, with $T_* = 10^4 \text{K}$ (hereafter T4), the nominal critical flux is much lower than for the T5 type, typically $J_{\text{crit}} \sim 30$ (e.g. Omukai 2001). In the T4 case, photodetachment of H^- , a precursor in the primary formation reaction for H_2 , causes suppression of H_2 -cooling, rather than photodissociation. This is due to the large IR flux near the photodetachment threshold ($h\nu \approx 1 - 2 \text{eV}$) in a T4 spectrum compared to

the T5 spectrum *for a fixed J_{21}* . However, as shown by Wolcott-Green & Haiman (2012), this can be misleading: the mass in stars must, in fact, be higher for a T4-type population to produce the same J_{21} as a T5-type. Thus, the lower value of J_{crit} for the soft T4 spectrum makes it more difficult, rather than easier, to suppress H_2 -cooling.

The main goal of this paper is to investigate the H_2 -cooling in the case of a “realistic” Pop II spectrum for the incident radiation field, rather than an idealised spectrum such as a blackbody or power-law. A single flux, J_{crit} , is sufficient for determining the cooling history for a blackbody (power-law), because for a given blackbody temperature (exponent), there is a fixed ratio of flux in the LW bands to the flux at the photodetachment threshold (0.76eV). However, for more realistic spectra from population synthesis modeling, it is necessary to consider separately the H_2 -photodissociation (k_{LW}) and H^- -photodetachment rates (k_{H^-}), and their evolution over time.

We show in § 3 that *there is, in general, a “critical curve,” rather than a single J_{crit}* , for determining whether H_2 -cooling is suppressed and thus whether the halo is a candidate for a DCBH. This critical curve is a line in the k_{LW} vs k_{H^-} plane, and is independent of the spectral shape. We consider a range of population synthesis model spectra from STARBURST99 and show how the results compare, with respect to the critical curve, with results from blackbodies ($T_* = 10^4 - 10^5 \text{K}$). We also provide an updated criterion for determining whether H_2 -cooling is suppressed, as a fitting formula for the critical curve.

The non-existence of a single J_{crit} and its importance for time-evolving spectra from population synthesis models has also been pointed out recently by Agarwal & Khochfar (2015) and Agarwal et al. (2016). These studies, as well as Sugimura et al. (2014) have investigated the relative importance of k_{LW} and k_{H^-} from STARBURST99 and from blackbody spectra in suppressing H_2 -cooling. We here improve on these studies by computing the H_2 -photodissociation rate, summing over all relevant LW lines, rather than assuming that the spectrum is flat in the LW bands, or taking an average of the LW flux. We show that both previous approximations, though computationally efficient, introduce significant errors in the photodissociation rate compared to our full frequency-dependent calculation.

This paper is organised as follows: In § 2 we describe the details of our numerical modeling. We present our results using a variety of STARBURST99 models in § 3, along with an updated fitting formulae for both the critical curve and critical mass in stars. We briefly discuss the results and implications of our work for future studies, and offer our conclusions in § 4.

2 MODELING

2.1 One-Zone Model

We use a one-zone model to follow the thermochemical history of primordial gas in a collapsing atomic cooling halo. This model has been shown to mimic the evolution found in three-dimensional hydrodynamical simulations very well (Shang et al. 2010, hereafter SBH10) and is described in detail in, e.g. Omukai et al. (2008). We briefly summarize the

² Recent simulations (Regan et al. 2014) have suggested that fragmentation might occur at spatial resolution higher than currently numerically feasible. On the other hand, even if fragmentation occurs, a supermassive star may still be the natural outcome, as long as H_2 cooling is disabled, owing to the rapid migration and coalescence of the central fragments (Inayoshi & Haiman 2014; Hosokawa et al. 2016).

model here and highlight a few important updates we made to the chemistry network.

The one-zone model prescribes a homologous spherical collapse, in which the dark matter evolution is that of a top hat overdensity with turnaround redshift $z_{\text{ta}} = 17$ and ρ_{DM} constant after virialization. The timescale of collapse is taken to be the free-fall time. Using the solver LSODAR, we follow the thermal and chemical evolution of initially primordial gas, with nine chemical species included: H , H^+ , He , He^+ , He^{++} , H^- , H_2^+ , H_2 , and electrons. Deuterium species are not included, as they do not affect our results at the temperatures of interest here, which are too high for HD-cooling to be important. Compressional heating as well as photochemical heating and cooling processes are included as detailed in SBH10.

We have made several updates to the one-zone model, most of which have not been included in previous studies (Agarwal et al. 2016, is an exception). We use the modified self-shielding expression provided by Wolcott-Green et al. (2011), which is more accurate for gas near the critical density, $n \gtrsim 10^3 \text{ cm}^{-3}$. The impact of a non-LTE ro-vibrational distribution is discussed in § 3.4. Wolcott-Green et al. (2011) showed that the column density approximation most often used in the one-zone model for the optically-thick k_{LW} overestimates shielding by about an order of magnitude in the density range of interest compared to 3D simulations. We therefore modify the column density as recommended in that study: $N_{\text{H}_2} = 0.25 \times \lambda_{\text{Jeans}} \times n_{\text{H}_2}$, which is half of the commonly used value. Here λ_{Jeans} is the Jeans length and n_{H_2} is the number density of molecular hydrogen. Though this is a somewhat crude fix, it more closely matches the results for optically-thick gas found in 3D hydrodynamical simulations. One caveat should be noted here: in general, H_2 self-shielding behavior will depend on the shape of the incident spectrum, since the shape determines the relative weights of the LW transitions. However, in practice, we find that the self-shielding function for a given SB99 spectrum differs very modestly from that for a flat spectrum, with errors typically of order a few per cent for young bursts, and not larger than $\lesssim 25$ per cent for the spectra considered here.

We have also updated some of the most important chemical rates which determine the H_2 abundance, based on the results of recent studies. These include the associative detachment rate ($\text{H} + \text{H} \rightarrow \text{H}_2 + \text{e}$; Kreckel et al. 2010), and the mutual neutralization rate ($\text{H}^- + \text{H}^+ \rightarrow 2\text{H}$; Stenrup et al. 2009). We have added several reactions to the one-zone chemistry network which have been shown to be important by, e.g. Glover (2015a,b). These include collisional dissociation of H_2 by neutral hydrogen through dissociative tunneling, the rate for which is provided by Martin et al. (1996) and the ionization of atomic hydrogen by H-H collisions and H-He collisions, using the rates from Lenzuni et al. (1991). The radiative recombination rate for H^+ is the Case B rate from Hui & Gnedin (1997) – appropriate for low-ionization fraction of gas collapsing in an atomic cooling halo (Glover 2015b) – rather than the Case A rate previously used in SBH10. We use the rate for radiative association from Abel et al. (1997), rather than that from Hutchins (1976) used by SBH10. The remainder of the chemistry network is the same as in SBH10 and provided in their Appendix.

Table 1. Summary of STARBURST99 model galaxy parameters. All assume a power-law IMF with exponent α and mass limits given below in units of M_{\odot} . Each IMF is run with metallicities $Z = 0.001, 0.004, 0.008 Z_{\odot}$.

Case	A	B	C	D	E
Limits	(1,120)	(10,120)	(30,120)	(30,500)	(100,500)
α	2.35	2.35	2.35	1	1

2.2 Model Spectra

We use the publicly available population synthesis package STARBURST99 (Leitherer et al. 1999, hereafter SB99) to generate spectra with a range of metallicities, IMFs, and ages. We use the UV line spectra provided by SB99 (at 0.3 Å resolution) for calculating the H_2 -photodissociation rate. Unfortunately, high-resolution spectra are not available for the full wavelength range required for all photochemical rates; therefore, for all continuum processes we use the SB99 spectra at lower resolution, which varies from (1-20 Å) over the relevant wavelengths.

We focus here on spectra for the SB99 “burst” models, in which a single population with specified mass, metallicity and IMF forms instantaneously and evolves over time, without any ongoing star formation. In the DCBH scenario, these are likely the most relevant, because the intense flux required for H_2 -cooling suppression must come from a very bright close neighbor, rather than from the cosmological background (see e.g. Shang et al. 2010; Dijkstra et al. 2008; Ahn et al. 2009; Agarwal et al. 2012, 2014; Regan et al. 2014; Habouzit et al. 2016). These studies show that the most likely candidates for DCBHs are within 1-2kpc of a bright source. As pointed out by Visbal et al. (2014), one promising scenario is that two atomic cooling (sub-)halos in very close proximity are nearly synchronised in their collapse, so that the first to form stars illuminates the other with a strong LW flux mostly from young, bright, massive stars. Visbal et al. (2014) and Regan et al. (2016) show that there are issues of photoevaporation if the collapsing DCBH candidate halo has been irradiated with a strong flux for $\gtrsim 20$ Myr; we therefore focus primarily on burst populations with ages up to 20 Myr.

We summarize the IMF parameter choices for our SB99 models in Table 1. Each IMF is run at three different metallicities from $Z/Z_{\odot} = 0.05 - 0.4$, though for the direct collapse model, the lower end of the range is more likely to be relevant, as the DCBH halo must be nearly pristine (see, e.g. Omukai et al. 2008), and is less likely to remain so with a highly enriched near neighbor.

The specific luminosities at the Lyman limit ($L_{13.6}$ in units $\text{erg s}^{-1} \text{ Hz}^{-1} M_{\odot}^{-1}$) output by SB99 are converted to J_{21} by:

$$J_{21} = \frac{M_*}{16\pi^2 d^2} \times \frac{L_{13.6}}{10^{-21}}, \quad (1)$$

where M_* is the total stellar mass of the SB99 burst galaxy and d is the distance from the illuminating halo.

In Figure 1, we show an example SB99 spectrum with metallicity $Z/Z_{\odot} = 0.05$ at $t = 10\text{Myr}$, as well as T4 and T5 blackbodies normalised to have the same luminosity at the Lyman limit. The frequencies of the H_2 LW transitions are

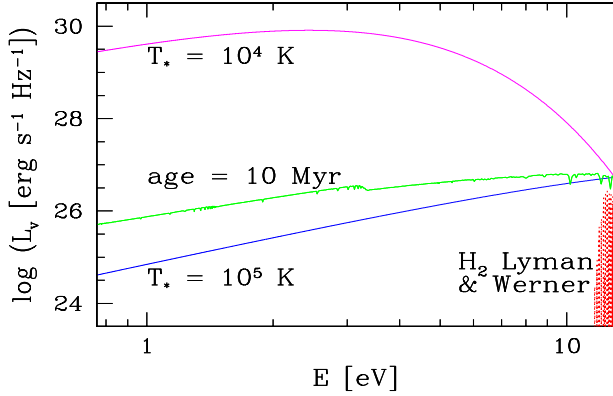


Figure 1. The spectrum of a STARBURST99 instantaneous burst model with stellar mass $M_* = 10^6 M_\odot$, IMF A, metallicity $Z/Z_\odot = 0.05$, and age $t = 10$ Myr is shown in green. Spectra of blackbodies with $T_* = 10^4$ (T4) and 10^5 K (T5) are shown, scaled to the same luminosity at the Lyman limit. Red (dotted) vertical lines show the Lyman-Werner band transitions (arbitrary units). We show the spectra in the energy range of interest, from the H^- photodetachment threshold, 0.76 eV, to the Lyman limit, 13.6 eV. The SB99 spectrum is much closer to T5 than to T4.

also shown for reference. As this figure illustrates, the SB99 spectrum is much closer to the T5 spectrum at the energies most important for H^- -photodetachment, 1-2 eV. In § 3 we discuss further the comparisons between SB99 spectra and blackbodies and the implications for H_2 -cooling.

2.3 H_2 -Photodissociation Rate

We calculate the frequency-dependent optically-thin H_2 -photodissociation rate for each of the SB99 models using the high-resolution UV spectra. Photodissociation occurs via the two-step Solomon process (Solomon 1965; see also Field et al. 1966; Stecher & Williams 1967), in which H_2 molecules are electronically excited by absorption of Lyman-Werner photons (900-1100 Å). Following excitation, ~15% of molecules are dissociated in subsequent radiative decay to the vibrational continuum of the electronic ground state, while all others return to a bound state via radiative cascade.

The rate of photodissociation of molecules from initial ro-vibrational state (v, J) is

$$k_{\text{diss}, v, J} = \sum_{v', J'} \zeta_{v, J, v', J'} f_{\text{diss}, v', J'}, \quad (2)$$

where $f_{\text{diss}, v', J'}$ is the fraction of molecules that are dissociated from the excited state (v', J') , provided by Abgrall et al. (2000). The “pumping rate” of H_2 from the ground state (v, J) to (v', J') is:

$$\zeta_{v, J, v', J'} = \int_{\nu_{\min}}^{\nu_{\max}} 4\pi \sigma_{v, J, v', J'}(\nu) \frac{J_\nu}{h\nu} d\nu; \quad (3)$$

where J_ν is the specific intensity of the SB99 spectra in the usual units and h is Planck’s constant. The limits of integration are from $h\nu_{\min} = 11.1$ eV to $h\nu_{\max} = 13.6$ eV. We use the data from Abgrall et al. (1993) to obtain the frequency-dependent Lyman-Werner absorption cross-sections $\sigma_{v, J, v', J'}(\nu)$.

The total H_2 -photodissociation rate depends on the ro-vibrational distribution of molecules, $f_{v, J}$:

$$k_{\text{LW}} = \sum_{v, J} k_{\text{diss}, v, J} f_{v, J}, \quad (4)$$

which in general can depend on the detailed thermochemical history of the collapsing cloud. For simplicity, we assume all molecules are in the ground vibrational state with a Boltzmann distribution over rotational levels (up to $J=29$). Although the critical densities for rotational levels $J \gtrsim 5$ are larger than in our models ($n_{\text{H}} \gtrsim 10^4 \text{ cm}^{-3}$), the populations in those levels are vanishingly small for a Boltzmann distribution at $\sim 10^3$ K. We further discuss the implications of a non-LTE ro-vibrational distribution in § 3.4.

2.4 Rate of H^- Photodetachment

The rate of H^- photodetachment is computed with the widely-used Shapiro & Kang (1987) fit for the cross-section data from Wishart (1979). This is convolved with the flux from a blackbody or SB99 spectrum:

$$k_{\text{H}^-} = 4\pi n_{\text{H}^-} \int_{0.76 \text{ eV}}^{13.6 \text{ eV}} \sigma_{\nu, \text{H}^-} \frac{J_\nu}{h\nu} d\nu. \quad (5)$$

Miyake et al. (2010) pointed out that a series of auto-detaching resonances above ~ 11 eV also contribute to the photodetachment rate; however, they find the additional suppression of the H_2 abundance is only $\lesssim 20$ per cent for blackbody spectra with T_{BB} up to 10^5 K, and we therefore do not include these resonant contributions to the rate.

3 RESULTS AND DISCUSSION

3.1 Approximate Photodissociation Rates

Due to the computational expense of calculating the frequency-dependent H_2 photodissociation rate as described above, nearly all previous studies have instead derived an approximate rate by assuming that the (incident) flux across the LW bands is flat. With the flux at 13.6 eV specified by J_{21} in the usual units, the optically-thin rate is then parameterised as

$$k_{\text{LW}} = 1.39 \times 10^{-12} \beta J_{21}. \quad (6)$$

By convention, the rate is calculated assuming a flat spectrum in the Lyman-Werner bands and β is usually defined as the ratio of the flux at a single LW frequency to the flux at the Lyman limit, $\beta = J_{\text{LW}}/J_{21}$. The most common choice is to define J_{LW} as the flux at 12.4 eV, the midpoint of the Lyman-Werner bands; we refer to this as β_{flat} (e.g. Shang et al. 2010). Alternatively, some studies define J_{LW} as the average flux in the LW bands (e.g. Agarwal & Khochfar 2015); we will refer to this as β_{avg} :

$$\beta_{\text{avg}} = \frac{1}{\Delta\nu_{\text{LW}}} \int_{\nu_{11.1 \text{ eV}}}^{\nu_{13.6 \text{ eV}}} J_\nu d\nu \quad (7)$$

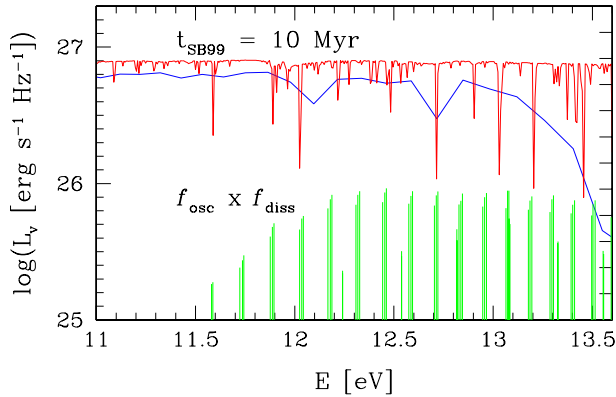


Figure 2. High- (red) and low-resolution (blue) spectra in the Lyman–Werner bands for a STARBURST99 model of an instantaneous burst with IMF A and $Z/Z_{\odot} = 0.05$ at 10 Myr. The Lyman–Werner transition strengths are shown in green. Because the absorption lines in the high-resolution spectrum overlap with the LW transition energies, significant errors can result from the assumption that the spectrum is flat in the LW bands, even when, as is the case here, the stellar population is relatively young and total absorption is modest.

These approximations save significant computational expense, avoiding integration over dozens or hundreds of LW lines, as described in the full rate calculation above. However, even in the idealised case of a 10^4 K blackbody spectrum, a non-zero slope of the spectrum in the LW bands can lead to errors in k_{LW} of a factor of two compared to the rate if the spectrum is assumed flat at 12.4 eV. Hotter blackbody spectra are flatter in the LW bands so the errors are smaller, and only a few percent for $T_{BB} = 10^5$ K. For more realistic spectra, however, such as those from population synthesis codes like SB99, both the non-zero slope as well as absorption features – e.g. O IV $\lambda 1035$, Ly β , C II $\lambda 1036$, and LW lines themselves (Leitherer et al. 1999) – near the LW transition frequencies can cause the rate derived from β_{flat} or β_{avg} to deviate significantly from frequency dependent (“true”) rate.

In Figure 2 we show examples of SB99 spectra (high and low-resolution) in the LW bands, overlaid with the 76 ground state LW transitions. (Relative transition strengths are shown by the product of the oscillator strength f_{osc} and dissociation fraction f_{diss} .) Because previous studies of the photodissociation rate have derived β_{approx} from the low-resolution SB99 spectra, we first compare the accuracy of these approximations using the low-resolution spectra in our full frequency-dependent rate calculation.

The results in Figure 3 show that β_{flat} (solid red curve) and β_{avg} (dashed blue curves) are good approximations for the early (of order 10 Myr) SB99 spectra which are relatively flat in the LW bands, compared to later times. Both overestimate the photodissociation rate by a factor of ~ 2 by 100 Myr and increasing thereafter, due to the significant dips in the low-resolution spectra near the Lyman-limit. We note that although the errors in these common methods of nor-

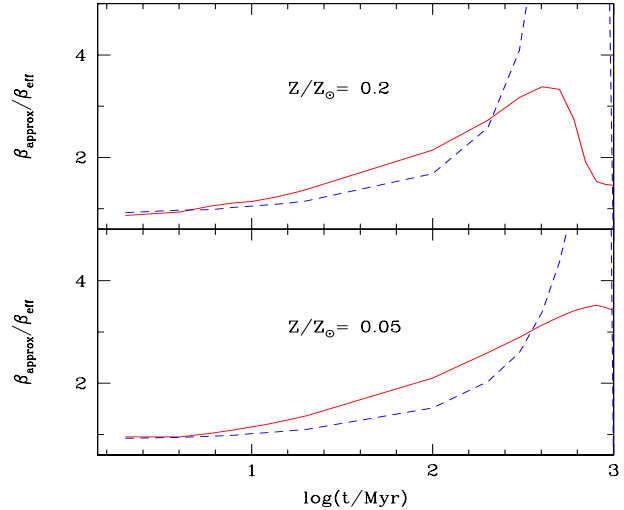


Figure 3. Ratio of the Lyman–Werner photodissociation rate, parameterised by the dimensionless parameter β (eq. 6), from an approximate method (β_{approx}) to the full, frequency-dependent calculation (β_{eff}). In all cases the spectrum is the low-resolution UV from a STARBURST99 instantaneous burst with metallicity as indicated on the figure. The dissociation rate assuming either the average flux in the LW bands (β_{av}) or a flat spectrum (β_{flat}) with $J_{LW} = J(12.4\text{eV})$ both overestimate the “true” rate by a factor of ~ 2 at 100 Myr after the burst and a larger factor for older bursts. This is due to the strong attenuation of the flux near the Lyman-limit (line blanketing), which is not captured by the approximations of flat spectra in the LW bands.

malizing are relatively small at early times, in the DCBH scenario, even factor of $\lesssim 2$ errors in k_{LW} and the corresponding critical flux leads to large errors in the predicted numbers of candidate halos (Dijkstra et al. 2008).

Note that, as shown in Figure 2, beyond resolving individual lines, the high-resolution spectra tend to have higher mean flux levels than the low-resolution spectra. These two effects can lead to significant differences in the predicted photodissociation rates. In Figure 4 we show a comparison of the (frequency-dependent) rates calculated using the high-resolution UV spectra (“ k_{eff} ”) with those obtained from the approximate methods (flat or average) and low-resolution spectra (“ k_{approx} ”). This gives an indication of the overall error made in most previous studies, which use the latter. In this case, the effect of (modestly) over-estimating β is counteracted by the smaller flux levels of the high-resolution spectra, and the upshot is the overall rate is underestimated by a factor of a few. We include the comparison only up to 20 Myr, after which the high-resolution UV spectra are no longer reliable (C. Leitherer, private communication).

3.2 Critical Curve

In general, H_2 dissociation, and therefore the thermal history, of gas in a primordial atomic cooling halo is controlled by two rates: H_2 -photodissociation by LW photons (k_{LW}) and H^- -photodetachment by IR photons (k_{H^-}), since H^- is an intermediate in H_2 formation. While a threshold flux, J_{crit} , has most often been used to determine whether H_2 -cooling should be suppressed, this can be misleading, and it

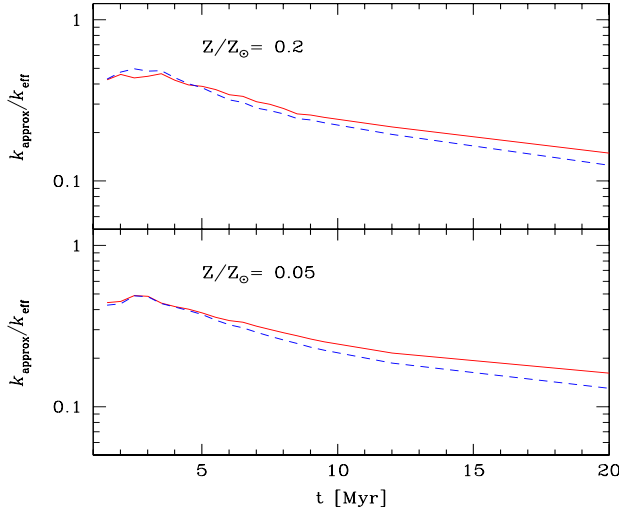


Figure 4. Ratio of the Lyman–Werner photodissociation rate from frequency–dependent calculation using the high–resolution UV STARBURST99 spectra (k_{eff}) to the rate using the low–resolution spectrum and normalizing assuming either (i) a flat spectrum with 12.4eV normalization (red solid line) or (ii) average flux in the LW bands (blue dashed line).

requires the computation of J_{crit} specific to each spectrum. J_{crit} values have been estimated in the literature for idealised spectra with fixed shapes, such as a blackbody or power-law, but have then subsequently been adopted for different spectral shapes, without re-computing the appropriate J_{crit} values (e.g. Agarwal et al. 2012; Dijkstra et al. 2014). For realistic, time–evolving spectra, such as those generated in population synthesis models, both k_{LW} and k_{H^-} need to be re-computed and specified to determine whether H_2 –cooling is suppressed. Although a corresponding J_{crit} can be computed, as well, this, as we have emphasized, is unnecessary and misleading, and has led to erroneous assumptions in previous works. We therefore propose to replace the “critical flux” with the spectrum-independent “critical curve,” as shown in Figure 5.

The solid curve in Figure 5 shows the minimum combination of k_{LW} and k_{H^-} required to keep the gas hot in our one–zone models. This curve results from the cooling behavior of the gas in our one–zone models, which follows the familiar bifurcated path: with a sufficiently strong radiation field, the H_2 –fraction remains too low for cooling to occur, and the gas is near the virial temperature of the halo throughout the initial stages of collapse (up to $n \gtrsim 10^7 \text{ cm}^{-3}$). Below the threshold, the H_2 fraction reaches $\sim 10^{-3}$, cooling the gas to $\sim \text{a few } \times 10^2 \text{ K}$. On the critical curve in Figure 5, for all points above (rightward) of the curve, H_2 –cooling is suppressed, while for those below (leftward) of the curve, H_2 –cooling occurs and the gas temperature falls below 10^3 K . *The curve itself depends only on the details of the one–zone model, and does not depend on the shape of the irradiating spectrum.* The location where each individual model spectrum falls relative to the critical curve does, however, depend on the spectral shape.”

For ease of comparison with previous studies, we have marked on the critical curve the positions of blackbodies

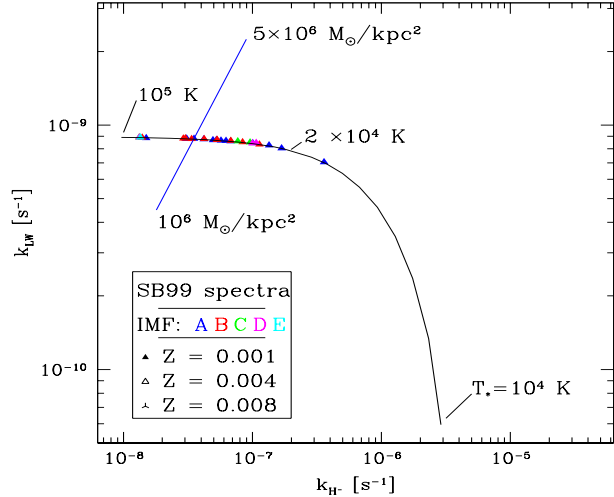


Figure 5. The “critical curve” (in black) shows the minimum combination of H_2 photodissociation and H^- –photodetachment rates required to prevent H_2 –cooling in an atomic cooling halo. Above and to the right of the black curve is the region in which the halo remains hot enough to be a candidate for a direct collapse black hole. Several points are marked with the temperature of a blackbody spectrum required to produce the ratio of the two rates along the critical curve. Each triangle represents the rates produced by a particular STARBURST99 model spectrum with metallicity and IMF as indicated in the legend. The (blue) diagonal line segment in the upper left shows the rates for SB99 models with varying stellar mass ($10^6 M_\odot$ at lower left and $5 \times 10^6 M_\odot$ at top right), for IMF “A” at 10 Myr after the burst and at a distance of 1 kpc. Depending on the assumed efficiency of star formation, this indicates a required (critical) halo mass of at least $10^8 M_\odot$ for the illuminating galaxy.

of several different temperatures. It is worth noting that all blackbodies with temperatures $\gtrsim 20,000 \text{ K}$ lie in the flat portion of the curve, i.e. where photodissociation is the dominant mechanism for suppressing H_2 –cooling, while H^- –photodetachment is only important for the coolest blackbodies considered, $\sim 10^4 \text{ K}$. While the T4 type has often been used in previous studies to approximate Pop II, the positions of the SB99 spectra on the critical curve underscore that it is not a good representation of Pop II; further, the increased fraction of mass in stars remains a problem for achieving H_2 –cooling suppression from populations with the softest (T4 type) spectra (Wolcott-Green & Haiman 2012).

The points in Figure 5 are the results of our one–zone model using individual SB99 spectra for the illuminating radiation field, each normalised with M_*/d^2 so as to coincide with the critical curve. SB99 bursts with all five IMFs and metallicities $Z/Z_\odot = 0.05 - 0.2$ are shown. While the SB99 spectra at early times ($\lesssim 10 \text{ Myr}$) and low–metallicity ($Z/Z_\odot = 0.05$) are comparable on the critical curve to higher temperature blackbodies, indicating that LW dissociation dominates the suppression of the H_2 abundance, the IR radiation becomes important before 20 Myr for models with modest metallicities ($Z/Z_\odot = 0.2$).

Our “critical curve” differs from that of Agarwal et al. (2016) due to our use of a reduced self–shielding column density, (see § 2), as discussed above and in Wolcott-Green et al.

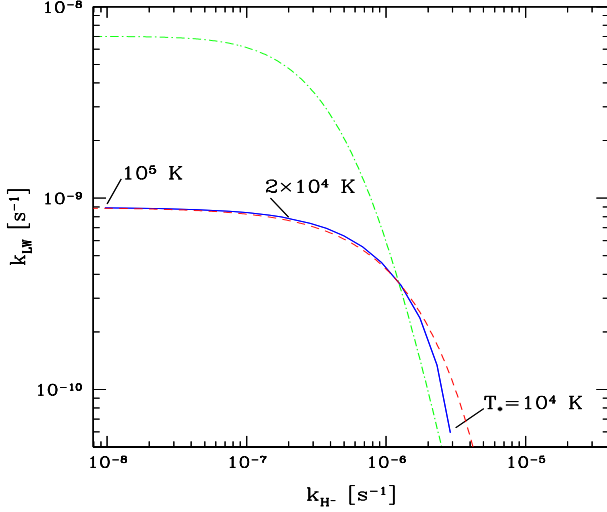


Figure 6. Our fitting formula (eq. 8) for the critical curve is shown in red (dashed), with the curve from our one-zone calculation in blue (solid). A fitting formula from a previous study (Agarwal et al. 2016) is shown in green (dot-dash).

(2011). For the SB99 spectra, our results also differ due to our frequency-dependent calculation of the photodissociation rate. Our k_{LW} is smaller in general, for a given model, than in other studies, since β_{flat} and β_{avg} overestimate the actual rate. Our results are broadly consistent with those of Sugimura et al. (2014), although, as previously noted, we have chosen not to explicitly use J_{crit} , as is done in their Figures 5 and 6. Again, the primary differences are due to our use of a reduced self-shielding column density, which yields a smaller J_{crit} for a given model; however, the overall trends in our results are broadly consistent.

In Figure 6 we show our new fitting formula (blue dashed curve) alongside the results of our one-zone modeling (red solid curve) and the fit provided by Agarwal et al. (2016) (green dot-dash curve). Our fit to the critical curve is given by:

$$k_{\text{LW}} = \frac{10^{-A}}{(1 + k_{\text{H}^-}/C)^D} \times \exp(-B * k_{\text{H}^-}/C), \quad (8)$$

with $A=9.05$, $B=0.95$, $C=1.6 \times 10^{-6}$, and $D=0.3$. This fit is accurate to a few percent for $k_{\text{H}^-} \lesssim 2 \times 10^{-6}$, corresponding to blackbody temperatures $\gtrsim 12,000\text{K}$ and the majority of SB99 results (which are leftward of that mark). It underestimates k_{LW} by a factor of two at $k_{\text{H}^-} = 3 \times 10^{-6}$ ($T_{\text{BB}} = 10^4\text{K}$).

3.3 Critical Star Formation in Illuminating Galaxy

In order to easily utilize our results in semi-analytic models and simulations of early structure formation, in Table 2 we provide the required stellar mass in an illuminating galaxy with a given IMF and metallicity, located at a distance d from an atomic cooling halo, to prevent H_2 -cooling: $\left(\frac{M}{d^2}\right)_{\text{crit}}$. This allows identification of DCBH candidate halo pairs without calculating individually the photodissociation and photodetachment rates. For two of our models (IMF A

Table 2. The required ratio of stellar mass and squared-distance $\left[\frac{M_*/10^6 M_\odot}{(d/\text{kpc})^2}\right]_{\text{crit}}$ for a starburst galaxy to prevent H_2 -cooling in a neighboring atomic cooling halo, obtained from the one-zone model.

IMF	age (Myr)	Z = 0.001	Z = 0.004	Z = 0.008
A	6	0.917	0.994	1.07
	10	1.96	2.36	2.74
	20	6.31	7.99	9.59
B	6	0.316	0.339	0.359
	10	0.746	0.893	1.04
	20	5.52	7.05	8.48
C	6	0.84	1.27	3.12
D	6	11.1	2.07	42.1
E	2	1.29	3.47	1.01

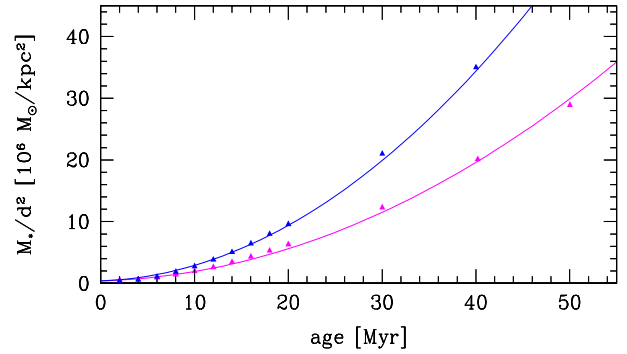


Figure 7. Our fitting formulae for $\left(\frac{M}{d^2}\right)_{\text{crit}}$ are shown (solid curves) with the data (triangles) from our one-zone models. In both cases we used IMF A for the SB99 spectra, with $Z = 0.001$ (0.008) shown in magenta (blue). The quadratic fit parameters are provided in § 3.3.

at $Z = 0.001, 0.008$) we also found analytic fits for $\left(\frac{M}{d^2}\right)_{\text{crit}}$, shown in Figure 7. These are quadratic fits with $a=0.011$ (0.02), $b=0.04$ (0.05), $c=0.4$ (0.4) for $Z = 0.001$ (0.008), with the usual convention used for the quadratic coefficients, $y = ax^2 + bx + c$. Both fitting functions are accurate to < 10 per cent up to 50 Myr.

3.4 Importance of Level Populations

The most significant simplification we made in this study is to assume the ro-vibrational level populations of H_2 are well described by a Boltzmann distribution in the rotational levels ($J = 0-29$) of the ground vibrational state ($v=0$). Deviations from LTE can significantly affect the self-shielding behavior of H_2 and therefore change the critical curve shown in Figure 5. In the early phases of gravitational collapse of an atomic cooling halo, the H_2 in $v=0$ would not have reached equilibrium, since the critical densities are already $n \sim 10^3 - 10^4 \text{ cm}^{-3}$ for the first few rotational levels.

At the relevant temperatures for the early collapse, i.e. a few thousand Kelvin, high J states ($J \gtrsim 5-10$) are negligibly populated, so this does not introduce significant errors in the optically-thin H_2 -photodissociation rate. As discussed in Wolcott-Green & Haiman (2011), however, the more levels

are populated, the less effective H_2 self-shielding becomes, so the optically-thick rate is more sensitive to the assumed distribution over ro-vibrational states. For example, in their study using the publicly available package CLOUDY to resolve level populations of H_2 , Richings et al. (2014) find differences compared to the optically-thick LTE rate of \sim a factor of a few for $T_{\text{gas}} = 5000\text{K}$ and $n_{\text{tot}} = 10^2\text{ cm}^{-3}$ at very high column densities, $N_{\text{H}_2} \gtrsim 10^{19}\text{ cm}^{-2}$ with much smaller errors at the relevant column densities for the early stages of collapse.

4 CONCLUSIONS

In most studies of the direct collapse black hole scenario, a single parameter J_{crit} has been used to delineate the threshold flux above which H_2 -cooling is prevented in an atomic cooling-halo. However, this single-parameter assumption can be misleading, as the value of J_{crit} depends on the spectral shape, and therefore needs to be re-computed for each incident spectrum. As long as the spectrum is assumed to have a fixed shape (in time), such as a blackbody or power-law, specifying the flux at a single frequency (e.g. the Lyman-limit) fixes all relevant photo-chemical rates. In a more general treatment, the ratio of the flux in the Lyman-Werner bands to that at the energies relevant for H^- -photodetachment ($\sim 1 - 2\text{eV}$), is dependent on the details of the spectrum, which depend on the mass function, metallicity, and age of the irradiating galaxy. Although a new J_{crit} could be computed for each case, we here emphasize that this is unnecessary, and advocate the use, instead of a two-dimension critical curve (Figure 5).

Using the population synthesis package STARBURST99 to generate realistic spectra, we investigated the relative importance of LW photodissociation and H^- -photodetachment in suppressing the H_2 abundance and thereby preventing cooling below the virial temperature of a halo. Very few studies have used spectra from population synthesis modeling, and those that have (Sugimura et al. 2014; Agarwal & Khochfar 2015; Agarwal et al. 2016) relied on simplifications to derive a LW photodissociation rate, rather than performing a full, frequency-dependent calculation. We show in § 3 that these simplifications overestimate the true photodissociation rate by a factor a few in the first $\sim 20\text{ Myr}$ of a burst.

We provide a fitting formula to the critical curve from our one-zone modeling (see Fig. 6 and Eq. 8), which includes important updates to the photochemical model and is accurate at the percent level. The resulting critical stellar masses (Table 2 and Figure 7) can be used directly in semi-analytic models and simulations of early structure formation.

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